

Benzonitrile
100-47-0 | DTXSID7021491

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.97e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.35e-01

Confidence level: 7.29e-01

Nearest Neighbors from the Training Set

Image not found

Allyl isothiocyanate

Measured: 2.02e-02

Predicted: 2.58e-02

Image not found

2,4-Pentadienenitrile

Measured: 1.90e-01

Predicted: 2.46e-01

Image not found

N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 1.34e-02

Predicted: 1.36e-02

Image not found

3-Butenyl isothiocyanate

Measured: 4.06e-03

Predicted: 4.19e-03